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APRIL 2, 1984

CHEMICAL & ENGINEERING

NEWS

French chemical industry finishes drastic restructuring
Page 22

PROCESS CONTROL

Closer ties with process simulation and design

Page 7

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Cover: Control loop being tuned at custom graphics console. Photo courtesy of Fisher Controls International

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CHEMICAL & ENGINEERING
NEWS
APRIL 2, 1984

News of the Week

■ **UN observers confirm the use of chemical weapons on Iranian ground forces in Persian Gulf war.** **Page 4**

■ **Polytechnic Institute of New York to offer master's program in imaging sciences and engineering.** **Page 5**

■ **First bits of data on Spacelab 1 experiments unveiled.** **Page 5**

■ **Racing car engine containing many plastic parts to debut in Connecticut race.** **Page 5**

■ **Atlantic Richfield sells its polypropylene operations to Cosden Oil & Chemical.** **Page 6**

■ **Crystallography technique may allow scientists to make movies of biological reactions.** **Page 6**

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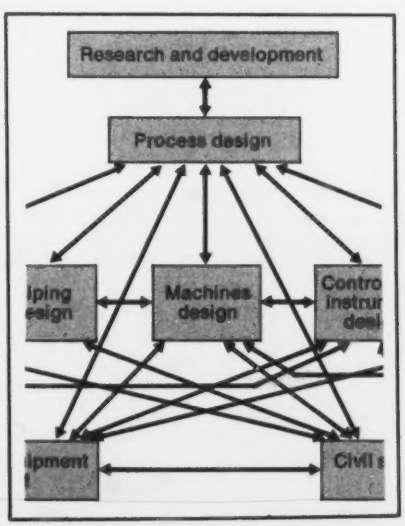


News Focus

Computerization is allowing further integration of chemical process control with simulation and design. **Page 7**

and piston pins, are made of its engineering resin Torlon, reinforced with carbon fibers. According to the company, Torlon is an injection-moldable thermoplastic polyamide-imide resin that can maintain structural integrity at temperatures up to 260 °C., under extreme load-bearing conditions.

The block, cylinder head, cam cover, and oil pan are made of Cycom, a composite made of woven Celion carbon fibers (from Celanese) impregnated with a thermosetting epoxy matrix resin (from American Cyanamid). Crankshaft, camshaft, combustion chambers, cylinder liners, piston heads, valves, and valve springs are metal. The engine, which contains 68 lb of metal, 60 lb of resins, and 40 lb of fiber reinforcement, is about 200 lb lighter than conventional engines of comparable size.

Polimotor president Matthew Holtzberg points out that reciprocating parts made of the light plastic generate lower inertial forces than do similar metal parts. The result, he claims, is 10% more available horsepower and a 12% cut in fuel use, compared to conventional engines.

Amoco and Polimotor note that the engine is still far too expensive for mass production; however, the current tests eventually could translate into improvements in passenger car engine design. □

Arco completes retreat from major polyolefins

Atlantic Richfield's shedding of major chemical operations now takes it virtually out of polyolefins. After recently bowing out of polyethylene, Arco now plans to leave polypropylene. The prospective buyer is Cosden Oil & Chemical, part of American Petrofina. For Cosden, a large producer of polystyrene, the move is a major diversification.

Cosden would be entering polypropylene production in the midst of a strong upturn in the thermoplastic. The rebound follows several years of poor business resulting from recession and overinvestment by new entries. The newcomers include Arco, which bought its plant from Diamond Shamrock in 1977 and then expanded it.

Cosden to start with 9% of polypropylene capacity

Millions of lb per year	Capacity
Cosden Oil & Chemical (American Petrofina)	470
Eastman Kodak	140
El Paso	370
Exxon	450
Gulf Oil	400
Himont	1320
Internorth	200
Phillips Petroleum	200
Shell Oil	600
Soltex Polymer	200
Standard Oil (Ind.)	550
U.S. Steel	515
TOTAL	5415

Sources: SRI International, industry estimates

Last week Arco and Cosden signed a letter of intent covering the polypropylene plant sale, which a Cosden spokesman says is expected to be closed in 90 days. The plant is at La Porte, Tex. Nameplate capacity after various expansions now is about 470 million lb per year.

The sale is subject to a definitive agreement, approval by the boards of directors of American Petrofina and Arco, and government agency approvals.

Cosden's move into polypropylene comes in a fast-rising market. In 1983, production topped 4.4 billion lb, up 28% from 1982, according to the Committee on Resin Statistics of the Society of the Plastics Industry. December 1983 production, the latest month for which data are available, was up 25% over December 1982.

The sale of its polypropylene continues a strategic about-face for Arco, which had built up strongly in polyolefins in the late 1970s. Earlier this year, Arco completed sale of its high- and low-density polyethylene plants at Port Arthur, Tex., to National Distillers.

Arco is now out of polyolefins except for a specialty polybutadiene plant. The reason for the current sale, says Arco Chemical vice president Bob G. Gower, is that the polypropylene unit is "not strategically critical" to the company, and the divestment will allow resources to be devoted to other projects. □

X-ray method may film biological reactions

Scientists at Cornell University have developed an x-ray crystallographic method that may someday allow them to make "movies" of biologically important reactions by piecing millisecond images together [*Science*, **223**, 1423 (1984)].

Using a 70-year-old and largely neglected technique called Laue diffraction and the intense x-ray beams from the Cornell High Energy Synchrotron Source (CHESS), the researchers have acquired structural data from horse methemoglobin and bovine intestinal calcium binding protein in times as short as 450 milliseconds. Further improvements may shorten times at least to 10 milliseconds. Such times would be short enough to study molecular changes during recombination of hemoglobin with carbon monoxide after laser photolysis or release of calcium from the binding protein.

The method was worked out by biochemistry professor J. Keith Moffat, senior research associate Doletha Szebenyi, and CHESS operations manager Donald Bilderback. Their research was supported by the National Institutes of Health.

Laue diffraction uses a broad spectrum of x-rays rather than the monochromatic x-rays used in conventional single-crystal studies. Spots on photographic film are due to wavelength rather than angle of incidence, allowing use of more light and eliminating the need to rotate the crystal to collect light.

The Cornell team will try to improve the method by using three to seven times the current in the synchrotron as in the present work. It also will use what is called a wiggler rather than a bending magnet to intensify x-rays. Collection efficiency will be improved by using transmission mirrors instead of absorption filters. And x-rays will be passed through helium rather than air to eliminate absorption by air. □

Chlor-Alkalies Come Back Strong From Recession

Demand, prices are up again for chlorine, caustic soda, and soda ash, but long-term outlook is slower growth than in recent years

Bruce F. Greek, C&EN Houston

The chlor-alkali industry staged a major comeback during 1983. It likely will continue to improve this year, but it could be a long time getting back to historical record levels of production and profitability.

A strong recovery for polyvinyl chloride last year gave chlorine the lead in both production upturn and price improvement over the other two major chlor-alkalies, caustic soda and soda ash. Caustic soda followed as the year ended and soda ash got on the bandwagon just recently.

Unfortunately, the recovery occurred in two steps for the chlor-alkalies as it did for most other products. First, demand rose substantially. Then prices followed. For some months, these products were sold at prices well below current ones, even though production then was just slightly lower than it is now.

For example, chlorine production rose 8.5% in 1983 and likely will grow 4 to 5% this year. The value of chlorine produced, which reflects both increased physical volume and higher selling prices, climbed about 18% in 1983. This year the value could be up 75% over last year because fall 1983 price increases and more recent ones will apply for the whole year.

Key Chemicals

Production of caustic soda, chlorine's coproduct, also likely will rise 4% or more this year. Like chlorine, the big gain in demand for caustic stems from chemicals manufacture, which accounts for about half of caustic's market. List price of caustic is presently about $240 per ton and deep discounting seems to have abated.

Prices in a demand downturn fall more quickly than they rise in a recovery. So these products didn't and probably won't get all the income so badly needed at a critical time. This situation seems almost unavoidable in the future when another recession could bring growth to a halt.

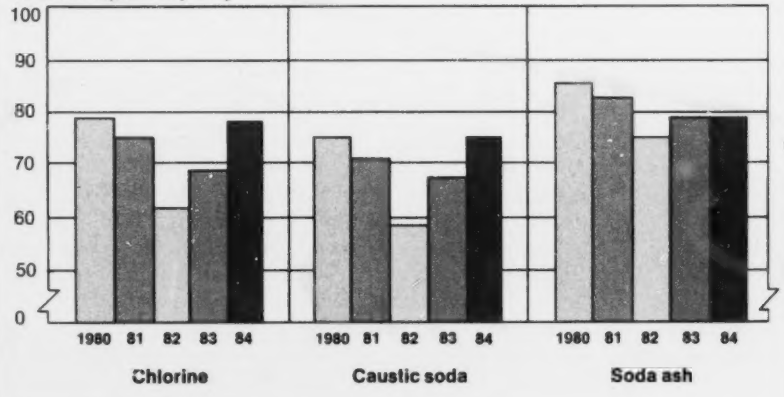
The long-term outlook for the chlor-alkali industry is for lower growth. Growth in 1984 of 4 to 5% for chlorine and caustic soda and 2% for soda ash could be viewed as good years for these products. Based on an analysis of the chlor-alkali industry by Consulting Resources, Roger Shamel, president of the company, forecasts long-term growth for chlorine and caustic soda at 1 to 2% per year and for soda ash 2 to 3% a year. This slow growth means a continuation of the loss of share of production by the U.S., now at about 30% of world production, according to Shamel.

This continuing decline in U.S. share of production could be accelerated by more plant closings. Except for soda ash, capacity declined in both 1982 and 1983, and it seems quite certain to decrease in 1984 and beyond.

No expansions of capacity, including that to make or recover soda ash, seem likely for a long time in the face of current demand forecasts. Investment money that does go to chlor-alkalies will be earmarked to improve process efficiencies, a major concern as the result of an order of magnitude increase in energy costs in the past decade.

For details of the near-term outlook for these major chlor-alkalies, see the following pages.

Capacity use will remain below 80% in 1984



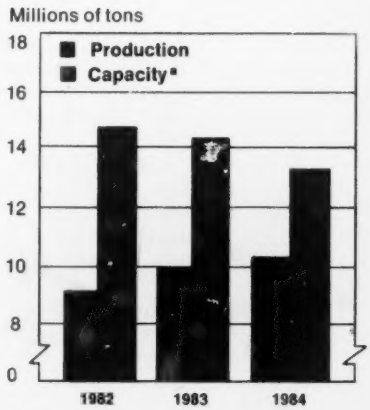
Sources: Industry and C&EN estimates, Chlorine Institute, Bureau of Mines

Chlorine

Cl_2

- ***Production recovering***
- ***Capacity down***
- ***Prices up strongly***

PRODUCTION/CAPACITY



a First quarter.

HOW MADE

Electrolysis of NaCl brine; recovery from hydrochloric acid; coproduct with metals; electrolysis of KCl brine

MAJOR DERIVATIVES (U.S.)

Ethylene dichloride 20%, other C_2 derivatives 10%, C_1 derivatives 10%

MAJOR END USES (U.S.)

Organic chemicals and plastics 65%, pulp and paper 15%

FOREIGN TRADE

Exports and imports—100,000 to 200,000 tons per year

PRICES

List prices $195 per ton and higher

COMMERCIAL VALUE

$2 billion for production, 1984

Currently U.S. producers of chlorine are enjoying a recovery from the recession of 1982. Gains in production forecast for this year, however, will not be so good as they were in 1983. But producers who stuck it out during the severe downturn may begin to show some profit this year as both selling prices and production are up substantially.

In 1984 production of chlorine likely will increase at least 4% to 10.4 million tons from last year's level. Output in 1983 was up 8.7% from the recent historical low of 9.2 million tons in 1982.

Surprises in chlorine production also might occur during 1984. The unexpected strength in the economy could mean a greater than previously forecast consumption of chlorine. As a result, production could rise 5 to 6% over 1983 to as high as 10.6 million tons.

Still, the robust production forecast for this year will be well below the record set in 1979 when production was nearly 12.3 million tons. Obviously, some years will be needed before output exceeds this record if growth rates hold at 4 to 5% annually. If the economy sags again, however, holding average growth to about 3% annually, then the 1979 record might not be exceeded before 1990.

Even as production of chlorine rises, capacity to make it falls and probably will continue to fall. At the beginning of this year, capacity was estimated at about 13.4 million tons a year, down 1 million tons from the estimate a year earlier and down 1.4 million tons at the beginning of 1982.

Clearly, the recession took a heavy toll of chlorine capacity, almost all of it in the electrolysis of sodium chloride brine. What happened is that plants using this process that had been shut down were scrapped under the economic pressure of the recession. Large investments in old plants would have been needed to make process efficiencies high enough to compete with new plants built during the most recent round of capacity expansions in the late 1970s and early 1980s. At the low selling prices of chlorine that existed during 1982 and early 1983, such investments could not be justified.

Possibly such investments can't be justified even now, considering the substantially higher prices being received for chlorine. As a result, some additional obsolete chlorine capacity may be shut down and eventually scrapped. Chances therefore are good that the industry's capacity will be lower at the beginning of next year than it is now.

Because of the shut-down capacity, producers' estimates vary on the actual operating rate for chlorine plants. For example, if all of the capacity estimated to be operable at the beginning of 1984 were utilized to produce 10.4 million tons of chlorine this year, the operating rate would be about 78%. That is well up from the rate calculated the same way for 1982—14.8 million tons of available capacity as the year opened and a total production for the year of 9.2 million tons—for a rate of 62%.

During 1982 and 1983, some capacity was scrapped and quite a bit was shut down, but not scrapped. Even now as much as 1.5 million tons of capacity could be shut down, because industry sources put the rate of the plants operating at between 85 and 90%.

The current strength in chlorine production and in operating rates because of the capacity reduction has considerably strengthened chlorine prices. List prices are up $50 per ton from last year's levels. Selling prices probably are up even more as a result of reductions in discounts off list prices.

Prices of chlorine derivatives are up, too, indicating that chlorine users are able to pass on much of the chlorine price increases. Higher prices for these derivatives, such as polyvinyl chloride, are the result of a healthy recovery in demand. As might be expected, some in the industry say that prices for PVC have increased about 50%, whereas chlorine prices have risen 33%.

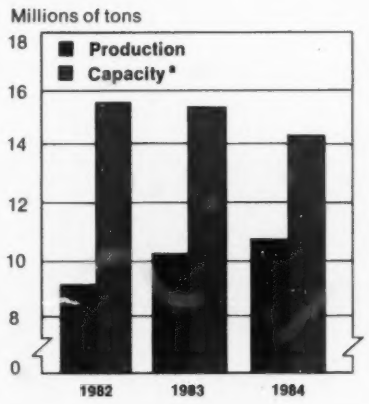
Increased demand, higher prices, generally more efficient plant operations, and improved profits will combine to make 1984 a much better year for chlorine producers than last year. No plans for capacity expansions are being made for certain, but some investment will go for membrane conversions to gain more efficiency. This year won't be so good as 1979, but it will definitely be better than the past three.

NaOH

Caustic soda

- ***Production rebounding***
- ***Capacity down***
- ***Prices turning up***

PRODUCTION/CAPACITY



a First quarter.

HOW MADE

Electrolysis of NaCl brine

MAJOR DERIVATIVES (U.S.)

None

MAJOR END USES (U.S.)

Chemical manufacture 50%, pulp and paper 20%, soap and detergents 5%

FOREIGN TRADE

Exports—down to less than 1 million tons in 1984, imports—rising to more than 400,000 tons

PRICES

List prices mostly $240 per ton; deep discounting now easing

COMMERCIAL VALUE

$2.2 billion for production, 1984

In a reversal of form from recent years, caustic soda (sodium hydroxide) is following the fortunes of chlorine, its coproduct in the electrolysis of sodium chloride brine. Both products are experiencing a continuing rise in production as demands improve with the economic recovery. As is the case for chlorine, the major gain in caustic demand comes from manufacture of chemicals, the natural result of the economic recovery.

Production of caustic in 1984 likely will be up at least 4% over production in 1983 to 10.7 million tons. If chlorine demand remains as strong as it has been in recent weeks and the rising demand for caustic continues, caustic output also could surprise forecasters. Finished caustic production also could be up 6 to 7% over 1983 production, possibly topping 11 million tons in 1984.

This production level, of course, still would be considerably below 1979's record output of caustic of about 12.8 million tons. At these forecast growth rates, it would take until about 1990 to match the 1979 record, assuming recessions do not interrupt the growth curve.

Caustic's price has improved and is currently about $240 per ton. Heavy discounting also has eased.

The industry's capacity to make caustic soda dropped roughly the same amount as chlorine capacity last year, or some 1 million tons, after a 400,000-ton drop in 1982. Now caustic capacity is about 14.3 million tons a year, perhaps a bit less as decisions have been made in the past two months to scrap plants that had been shut down previously. Again, as in the case of chlorine, caustic capacity probably will be lower at the end of this year than it was at the beginning.

Despite the close relationship of chlorine and caustic soda, small amounts of chlorine are made in other chemical processes, for example, as the coproduct of making caustic potash (potassium hydroxide), as the product of oxidation of hydrochloric acid, and as a by-product of the cracking of ethylene dichloride to make vinyl chloride. The only commercial route to caustic, on the other hand, is by electrolysis of sodium chloride brine.

However, not all caustic produced by this electrolysis process becomes reportable production. Depending on current economics, some quantities of caustic are not "finished" or concentrated from the cell liquor to commercial specifications but used in dilute form for alkalizing purposes in chemical processes. Such use further upsets production estimates based on stoichiometric production ratios of chlorine to caustic.

The nonchemical manufacturing uses of caustic also are sharing in the recovery. Pulp and paper manufacture, the largest such market with a 20% share of caustic demand, has been increasing its use for caustic even in the face of growing substitution of plastic films for paper. However, this use will not be a large gainer for caustic long-term.

The next largest outlet for U.S.-produced caustic is the export market. In 1983, exports rose slightly over 1982 but are still well down from 1981 when they amounted to about 1.3 million tons. For 1984, exports may decline again in the face of foreign competition.

As the worldwide economic recovery moves ahead, however, exports might hold steady or rise slightly as foreign producers of caustic find that their own markets are improving so much that they have less for export. New capacity for the electrolysis process in various countries plus economic changes makes exports difficult to forecast.

Imports, on the other hand, are expected to rise this year, probably topping 400,000 tons (they may have exceeded that quantity in 1983). Competition and the strong value of the dollar aid imports.

Other significant outlets for caustic are moving slowly, if at all. None will have much of an effect on caustic demand, one way or another.

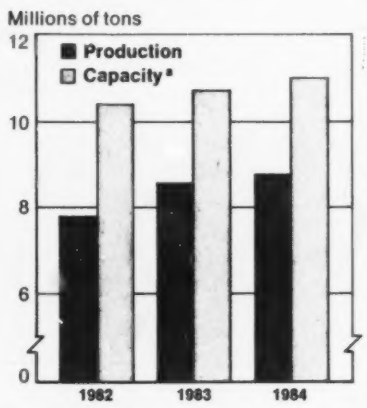
For this year then, caustic soda's fortunes will tag along with those of chlorine. If its demand improvement lags that of chlorine by about six months, that could keep it going a bit longer if chlorine demand should sag late in the year. On balance, caustic will contribute considerably to better profits this year, but probably to a smaller share than will chlorine.

Na_2CO_3

Soda ash

- ***Production at record***
- ***Capacity excessive***
- ***Price discounts cut***

PRODUCTION/CAPACITY



a First quarter.

HOW MADE

Recovered from trona ore or brine; synthesized from salt and limestone using ammonia

MAJOR END USES (U.S.)

Glass (containers and flat) 55%, chemical manufacture 20%, pulp and paper 5%, soap and detergents 5%

FOREIGN TRADE

Exports—easing to about 1.5 million tons in 1984, imports—negligible

PRICES

List price $84 per ton at Wyoming mines; discounts about $11

COMMERCIAL VALUE

$650 million for production, 1984

Soda ash producers are looking at a different year than are chlorine and caustic soda producers.

This year, production of soda ash may rise slightly, possibly 1 to 2%, signaling an end to the substantial demand recovery fueled by exports in 1983. The latest chlor-alkali price action, that of a reduction in temporary voluntary allowances (TVA) on list prices for soda ash, will be less helpful to profit margins than will be those initiated earlier for chlorine and caustic soda.

Soda ash demand and, in turn, production during 1983 depended heavily on the export market. Exports ballooned last year to more than 1.6 million tons, or some 19% of U.S. production. They were up about 500,000 tons over 1982 exports.

The recovery in the U.S. economy accounted for the remaining 200,000 tons of production growth for this chemical. With the strong surge and competitive pressures on the container market from plastics abating following the recovery, U.S. consumption of soda ash may grow slightly or even decline a bit in 1984.

Production, too, is a bit uncertain at this time, with forecasts for this year ranging from slight increases to declines. Optimists believe exports will rise again by a small amount, and that the slight rise in consumption will result from continued strong demand for flat glass by the housing and automobile industries and delays in the forecast growth of plastic containers at the expense of glass containers, primarily because of technical problems in making the containers as economically as expected. Glass currently accounts for more than half of the soda ash consumed.

Both the chemical and paper industry demand for soda ash will at least match that of 1983, with strong possibilities of an increased 100,000 to 200,000 tons going to these uses if caustic soda costs keep rising. These markets rank next to glass in importance among uses of soda ash.

As for exports, although the big increase in shipments of soda ash to China may be over for the near term, increased exports to a variety of other countries could add another 100,000 to 200,000 tons to demand for U.S.-produced soda ash.

Pessimists forecast that U.S. consumption of soda ash will slip 3 to 5% this year, or about 200,000 tons. This is because of the inroads of plastics into container markets, as well as a slowing of the rate of the economic recovery.

Exports of soda ash may hold at about 1.5 million tons through aggressive selling even as exports to China slow some. The worst-case scenario calls for a decline in production of about 200,000 tons this year. More likely would be a match of 1983 production with some small increase in inventories.

A more reasonable forecast for this year may be a 2% increase in soda ash production to about 8.7 million tons. This gain would be significantly lower than what is expected for chlorine and caustic soda.

Nameplate capacity to produce soda ash totals about 11 million tons a year of both natural and synthetic. No capacity expansions are in the works and even debottlenecking probably will be minor during 1984. Operation of this capacity will run at a 79% average for 1984. This rate will be a bit higher than a couple of years ago, but it still will not be at a level that could mean high plant efficiency and good profitability.

Slightly higher production, no new capacity, and considerable reduction in inventories during much of 1983 are factors that led to the reduction of the $15-per-ton TVA disclosed in early March. The reductions in the TVA vary a bit with location. Most important, however, is that the net list price for bulk material at the Green River, Wyo., location goes to $73 per ton. This price increase and possibilities of others later in the year have made soda ash producers, who have been struggling with limited profitability for some time, a bit more optimistic.

Although the big jump in demand may be over for now, soda ash fortunes improved in 1983 and seem to be continuing to improve as the first quarter of 1984 ends. If glass container consumption of soda ash doesn't fall too fast, a stabler demand and price situation could be beginning.

University Research Costing Changes Urged

Grant agencies and universities alike have been worried the past few years about the rapidly increasing proportion of research funds used to pay for expenses other than direct costs of research. These indirect research costs have attracted Congress' attention as well, and now the General Accounting Office has issued a long-delayed report that recommends, among other things, a fixed allowance for indirect costs at large universities.

In preparing the report, GAO looked mostly at grants made in 1981 and 1982 by the National Institutes of Health, which distributes about half the federal funds for health research and development and is considered the example for the rest of the federal programs. The investigative agency took a detailed look at 82 of the 200 or so universities that receive large amounts of NIH grants (more than $3 million annually) and tried to ascertain why each asked for the overhead that it did. These schools received $601 million from NIH in 1982, of which 32% was for indirect costs.

Specifically, GAO determined that, at NIH, indirect costs had risen from an average of 21% of cost of extramural research grants to 30% in the decade 1972–82. These funds are supposed to pay for university administration expenses, maintenance expenses, operation of facilities, and depreciation and use allowances. The rate of indirect costs as a proportion of the research grant is determined by each university for its specific circumstances according to instructions set forth in the Office of Management & Budget Circular A-21.

Proportion of NIH grants going to indirect costs has risen steadily

$ Thousands	Total grant costs	Total indirect costs	% of indirect costs to total costs
1972	$ 808,106	$166,243	20.6%
1973	799,665	185,587	23.2
1974	985,738	240,191	24.4
1975	1,000,496	258,936	25.9
1976	1,444,630	386,164	26.7
1977	1,320,302	359,140	27.2
1978	1,529,086	416,093	27.2
1979	1,844,001	512,279	27.8
1980	2,050,074	586,306	28.6
1981	2,224,138	655,143	29.5
1982	2,300,534	689,855	30.0

Source: General Accounting Office

In its report, GAO probed what the Department of Health & Human Services (of which NIH is a part) was doing to slow the growth of indirect charges, how well HHS was documenting the requests for increased indirect cost payments, and how often audits were done at universities and how these were used.

GAO had a problem when it came to verifying just why universities asked for large—more than 10%—increases in indirect costs. Much of the time there was no written explanation in the file for such a rise. And the largest area of increase was for departmental administration, an area in which it is impossible to segregate teaching from research from administration performed by the scientist. Estimates for time spent on different tasks given HHS negotiators by university administrators are very subjective and difficult to question therefore, and HHS usually accepts the request if it follows the OMB guidelines.

One way to verify the need for the indirect costs requested is to perform an audit of the university's system. However, that's not done very frequently. During a five-and-a-half-year period, GAO found that only 50 indirect cost audits had been performed by HHS on educational institutions. It also was determined that HHS was able to do only about half the audits requested by its grants negotiators. The department says it needs to devote more of its audit resources to the bigger programs like social security, medicare, and medicaid.

But where audits were done, significant amounts of indirect costs were not accepted. GAO says of 41 audits, which discussed $515 million in indirect expenses, the auditors refused to accept $64 million, or 12.5% of the request. The unwritten assumption is that if more audits could be performed, the indirect costs problem would be reduced considerably.

Of course, universities are correct in trying to recover their expenses for government-sponsored research. One reason for the increases was the inflation of the late 1970s, and higher administrative costs because of federally mandated social programs like affirmative action, pension benefits, and equal opportunity employment. Universities also have increased the sophistication of accounting methods trying to maximize their indirect cost requests.

To try to bring these costs down, the Administration proposed in 1982 that HHS cut indirect cost requests 10% across the board, but Congress refused to allow such a move. GAO is recommending that OMB revise Circular A-21 to establish a fixed allowance for indirect costs at large universities. This would cover all indirect expenses and could possibly vary from university to university depending on circumstances. HHS already has made some effort to control these costs, GAO reports. This includes asking grantees to justify increases in indirect costs in writing and a move to having more audits done by nonfederal auditing agencies.

The fixed rate concept already has some acceptance at other agencies and is being studied at HHS for NIH grants. And it is one of the savings suggestions made by the Grace Commission in its review of federal spending practices. Still, there is resistance to major changes in the system in Congress, where indirect-cost recovery is viewed by some as an important source of income for financially troubled universities. □